EMSP COLLABORATIONS

Research results are not always directly transferred to a specific end-user. Collaborations or interactions between EMSP researchers and others occur that increase the body of knowledge in a specific area as a direct result of EMSP funded research. This comes in many forms:

- 19 Consulting - provide advice or technical expertise
- 6 Joint interaction - researcher and end-user in joint interaction
- 6 Mission directed - project direction provided by end-user
- 10 Program interaction - researcher to researcher interaction
- 1 Unclassified.

This section describes the reported collaborations that have occurred within the EMSP. Numerous other less formal collaborations occur during the EMSP topical and national workshops. Many of these are anticipated to mature into the research partnerships and research transfers reported elsewhere in this document.

Project: 54506

Title: Acid-Base Behavior in Hydrothermal Processing of Wastes
PI: Dr. Keith P. Johnston *Institution:* University of Texas at Austin

Description: To develop this new branch of acid-base chemistry in water above 325?C and to achieve a breakthrough which could make hydrothermal oxidation a successful technology for the DOE, the objectives of this project are to develop a fundamental molecular understanding of the thermodynamics of ion solvation and acid-base equilibria and how they affect metal-ion complexation and salt solubility and to use this information to develop easily implemented, molecular-based models. Working with LANL on an experiment treating tank waste with high temperatures.
Collaboration Type: Joint interaction
Collaborator: Steve Buelow
Collaborating Organization: Los Alamos National Laboratory

Project: 54546

Title: Engineered Antibodies for Monitoring of Polynuclear Aromatic Hydrocarbons
PI: Dr. Alexander E. Karu *Institution:* University of California at Berkeley

Description: The objective of this project is to use molecular biological techniques to derive a set of antibodies with useful affinities and selectivities for recovery and detection of polynuclear aromatic hydrocarbons (PAHs) in environmental and biological samples. The long-term goal is to develop immunodetection methods that will be useful in biomarker research and regulatory monitoring of PAHs. Collaboration with Dr. Tuan Vo-Dinh at ORNL to identify sensor system and demonstration.
Collaboration Type: Mission directed
Collaborator: Dr. Tuan Vo-Dinh
Collaborating Organization: Oak Ridge National Laboratory

Project: 54656

Title: Mixing Processes in High-Level Waste Tanks
PI: Dr. Per F. Peterson *Institution:* University of California at Berkeley

Description: Flammable gases can be generated in DOE high-level waste tanks. This project is a concentrated effort to develop models and a numerical tool to mechanistically predict mixing processes in large waste-tank volumes, where mixing processes can be driven by hot and cold vertical and horizontal surfaces and injected buoyant jets. General Electric is funding a doctoral student to work on this project.
Collaboration Type: Consulting
Collaborator:
Collaborating Organization: General Electric

Project: 54672

Title: Radiation Effects in Nuclear Waste Materials
PI: Dr. William J. Weber *Institution:* Pacific Northwest National Laboratory

Description: Requested to assist in evaluating potential radiation-induced failure of protective glass globes for lights in the in-tank camera systems for Tank 101-SY at Hanford. Unexplained failure of two globes had raised some safety concerns. Working with Lockheed Martin Hanford Co. staff, an interim testing program was designed for the protective glass globes, a procedure to minimize potential failure (change globes frequently) was advised, and some preliminary measurements and evaluations were conducted on irradiated globes. No permanent solution was developed as yet.
Collaboration Type: Consulting
Collaborator: Scott M Werry
Collaborating Organization: Lockheed Martin Hanford Co.

Description: The effects of radiation from the decay of radionuclides in nuclear waste and other nuclear materials may potentially impact the long-term performance and stability of nuclear waste forms and stabilized nuclear materials. Using experimental and computer simulation approaches, this project endeavors to develop the underpinning science and models necessary to assess the effects of radiation on the performance of glasses and ceramics designed for the immobilization of high-level tank waste and stabilized nuclear materials. Collaborations with N.J. Hess, B.D. Begg, L.R. Corrales, H.L. Heinisch, and R.E. Williford at PNNL and with S.D. Conradson at LANL.
Collaboration Type: Program interaction
Collaborator: N.J. Hess, B.D. Begg, L.R. Corrales, H.L. Heinisch, and R.E. Williford; S.D. Conradson
Collaborating Organization: Pacific Northwest National Laboratory; Los Alamos National Laboratory

Project: 54679

Title: Architectural Design Criteria for F-Block Metal Ion Sequestering Agents
PI: Dr. Benjamin P. Hay *Institution:* Pacific Northwest National Laboratory

Description: Critical tasks in the cleanup of U.S. Department of Energy (DOE) sites include processing radioactive wastes for disposal in long-term storage, remediation/restoration of environmental sites resulting from radioactive contamination, and decontamination/decommissioning of nuclear facilities.Because the radioactive components, most of which are metals, are typically present in very low concentrations, it is desirable to remove them from the bulk of the contaminated source and concentrate them to minimize the volume of radioactive material destined for permanent subsurface disposal and thus minimize disposal costs. Over the past 50 years, much research has focused on the discovery of selective ligands for f-block metal separations; both neutral and ionic ligands have been examined. Despite past success in the discovery of ligands that exhibit some degree of specificity for the f-block metal ions, the ability to further control binding affinity and selectivity remains a significant challenge. The objective of this project is to provide the means to optimize ligand architecture for f-block metal recognition. Criteria for accurately selecting target ligands would result in a much more effective use of resources, thereby reducing the time and cost associated with metal-specific ligand development. Collaborations for each associated task are as follows:

Task: Synthesis and characterization of modified calixarene host molecules.
- Professor D. Max Roundhill, Department of Chemistry, Texas Tech University

Task: Crystal structure determinations.
- Professor Robin D. Rogers, Department of Chemistry, The University of Alabama

Task: Synthesis of amides and diamides, through a subcontract with Associated Western Universities to support a Postdoctoral Fellow, Dr. Robert Gilbertson, In Dr. Hutchison's group.
- Professor James E. Hutchison, Department of Chemistry, University of Oregon

Task: Provide structure-function data on catecholates and hydroxypyridonates.
- Professor Kenneth N. Raymond, Department of Chemistry, University of California at Berkeley

Task: Provide structure-function data on pyridine N-oxides.
- Professor Robert T. Paine, Department of Chemistry, University of New Mexico

In addition to interactions with University faculty, the project has supported a variety of visitors at Pacific Northwest National Laboratory through Associated Western Universities subcontracts, including:

- Dr. Pier L. Zanonato (Visiting Faculty, University of Padova, Italy) - calorimetry
- Dr. Bruce K. McNamara (Postdoctoral Fellow) - calorimetry, spectroscopy, solventextraction
- Dr. Omoshile Clement (Postdoctoral Fellow) - molecular mechanics
- Dr. Giovanni Sandrone (Postdoctoral Fellow) - quantum mechanics
- Dr. Rubicelia Vargas (Post Doctoral Fellow) - molecular mechanics and quantummechanics
- Dr. Jorge Garza (Visiting Faculty, Metropolitan Autonomous University -Iztapalapa, Mexico) - quantum mechanics

Collaboration Type: Program interaction
Collaborator: (see description)
Collaborating Organization: (See description)

Project: 54684

Title: Mechanism Involved in Trichloroethylene-Induced Liver Cancer: Importance to Environmental Cleanup
PI: Dr. Richard J. Bull *Institution:* Pacific Northwest National Laboratory

Description: EPA is using the data we have generated and a paper describing the mode of action for induction of liver tumors to revise their risk assessment on trichloroethylene. EPA continues to track our published results as this decision process reaches its conclusions. A separate step will be actions taken under the Office of Water to revise drinking water standards or CERCLA to modify clean-up standards that are derived from the revised risk assessments.
Collaboration Type: Consulting
Collaborator:
Collaborating Organization: EPA

Project: 54741

Title: Characterization of Contaminant Transport Using Naturally-Occurring U-Series Disequilibria
PI: Dr. Michael T. Murrell *Institution:* Los Alamos National Laboratory

Description: Consulted regarding uranium measurements at Rocky Flats by contractors for Rocky Flats and for the State of Colorado. We later received a small amount of funding to make some measurements for solar pond waters at Rocky Flats. The approach used was similar to that of our EMSP project.
Collaboration Type: Consulting
Collaborator: Dave Janecky
Collaborating Organization: Rocky Flats Environmental Technology Site, State of Colorado

Project: 54751

Title: High Fluence Neutron Source for Nondestructive Characterization of Nuclear Waste
PI: Dr. Mark M. Pickrell
Institution: Los Alamos National Laboratory

Description: The objective of the project is to research the basic plasma physics necessary to develop a high fluence neutron source based on the inertial electrostatically confined (IEC) plasma. An intense neutron source directly addresses the capability to characterize nuclear materials under difficult measurement conditions. Some of the applications for Environmental Management are the characterization of TRU wastes for WIPP, the measurements of residues prior to stabilization and disposal, the measurements of cemented or vitrified wastes, the measurement of spent nuclear fuel, and the measurement of high level wastes. Collaborations with the INEEL and the National Spent Nuclear Fuels Program to produce a neutron source for MDAS or other systems being developed by the INEEL.

Two commercial partners have applied for a license for the High Fluence Neutron Source, shown here in the laboratory. [see Project #54751]

Collaboration Type: Mission directed
Collaborator: Jerry Cole
Collaborating Organization: Idaho National Engineering and Environmental Laboratory

Project: 54828

Title: Processing of High Level Waste: Spectroscopic Characterization of Redox Reactions in Supercritical Water
PI: Dr. Charles A. Arrington, Jr. *Institution:* Furman University

Description: Collaborative research effort with LANL on the destructions of complexants and oxidation of chromium and technetium by hydrothermal processing in near critical or supercritical aqueous solutions.
Collaboration Type: Program interaction
Collaborator: Steven Buelow and Jeanne Robinson
Collaborating Organization: Los Alamos National Laboratory

Project: 54996

Title: Ionizing Radiation Induced Catalysis on Metal Oxide Particles
PI: Dr. Michael A. Henderson *Institution:* Pacific Northwest National Laboratory

Description: This project focuses on a novel approach for destroying organics found in high-level mixed waste prevalent at DOE sites. We have shown that ionizing radiation can be used to catalytically destroy organic chelating agents, such as EDTA, whose presence in high-level waste streams hinder the removal of radionucleii by ion exchange. Our studies have shown that gamma irradiation of titanium dioxide suspensions destroy the chelating ability of EDTA by decomposing it to smaller organic molecules. This has been demonstrated for both free EDTA in solution and for solutions of EDTA complexed to strontium. Present efforts are aimed at determining the mechanism by which EDTA is destroyed and the feasibility of using this process for treating high-level mixed waste.
Collaboration Type: Consulting
Collaborator: Abhaya K. Datye; Professor Miguel E. Castro
Collaborating Organization: University of New Mexico; University of Puerto Rico

Project: 55103

Title: Utilization of Kinetic Isotope Effects for the Concentration of Tritium
PI: Dr. Gilbert M. Brown *Institution:* Oak Ridge National Laboratory

Description: The objective of our work is to develop an electrochemically-based, cyclic process which can be used to remove tritium from contaminated water. We are developing methods for concentrating tritium from water based on large primary kinetic isotope effects in catalytic redox processes. H-T discrimination occurs in an oxidation step involving a transition metal oxidant and small organic compounds containing oxidizable C-H or C-T bonds. Tritium is incorporated in the organic compound by an electrochemical reduction process in the presence of tritium contaminated water, but the protio-derivative is kinetically favored in the oxidation half-reaction. As a result of a cyclic oxidation-reduction process, tritium is enriched in the organic compound. The organic compound is chosen so that it does not readily exchange the tritium with groundwater.
Collaboration Type: Consulting
Collaborator: C.H. Ho, Douglas J. Lemme, Leon Maya, and Frederick V. Sloop, Jr.; Poonam M. Narula and Thomas J. Meyer
Collaborating Organization: Oak Ridge National Laboratory; University of North Carolina at Chapel Hill

Project: 55110

Title: An Alternative Host Matrix Based on Iron Phosphate Glasses for the Vitrification of Specialized Nuclear Waste Forms
PI: Dr. Delbert E. Day *Institution:* University of Missouri-Rolla

Description: Certain high level wastes (HLWs) are not well suited for vitrification in borosilicate (BS) glasses because they contain components such as phosphates that are poorly soluble in a BS host matrix. The waste loading must be significantly reduced if one is to successfully vitrify such problematic wastes in a BS glass. Iron phosphate glasses offer a technically feasible and cost effective alternative to borosilicate glasses for vitrifying such HLWs. The main objective of the project was to investigate the atomic structure-property relationships, and glass forming and crystallization characteristics, of these iron phosphate glasses and glasses containing nuclear waste components. Other physical properties such as density and thermal expansion were studied. Collaborations for each associated task are as follows:

Task: X-Ray Absorption Spectroscopy (EXANES/EXAFS) at the Stanford Synchrotron Radiation Laboratory

- Drs. David Shuh, Jerry Bucher, N.M. Edelstein, and Corwin Booth, Lawrence Berkeley National Laboratory
- Dr. Pat Allen, Lawrence Livermore National Laboratory

Task: Neutron and High Energy X-Ray Scattering

- Drs. Marie-Louise Saboungi, Yaspal Badyal, and Dean Heaffner, The Division of Materials Science, Intense Pulsed Neutron Source, and The Advanced Photon Source, Argonne National Laboratory

Task: Raman Spectroscopy

- Dr. Marcos Grimsditch, Division of Materials Science, Argonne National Laboratory
- Dr. Andrea Mogus-Milankovic, Ruder Boskovic Institute, Croatia

Task: Electron Spin Resonance Studies

- Dr. David Griscom, Naval Research Laboratory

Task: Electrical properties (conductivity, loss, and dielectric constant)

- Dr. Andrea Mogus-Milankovic, Ruder Boskovic Institute, Croatia

Collaboration Type: Program interaction
Collaborator: (see description)
Collaborating Organization: (see description)

Project: 55205

Title: A Fundamental Study of Laser-Induced Breakdown Spectroscopy Using Fiber Optics for Remote Measurements of Trace Metals
PI: Dr. Scott Goode *Institution:* University of South Carolina

Description: Improved technologies are required by DOE for characterization and monitoring for site clean-up and waste processing applications. Especially needed are field deployable methods and devices of real-time monitoring. Matrices of interest to the DOE are soils, slurries, and aqueous and non-aqueous solutions. Laser-induced breakdown spectroscopy (LIBS) is a useful method for determining the elemental composition of solids. The objective of this project is to determine the optimal excitation and collection conditions and sampling times for metal contaminants in different matrices, and an understanding of the strengths and limitations of using fiber optics for LIBS sampling. PI is in the process of establishing a collaboration with EMSL.
Collaboration Type: Unclassified
Collaborator:
Collaborating Organization: Environmental Molecular Sciences Laboratory

Project: 55229

Title: The No_x System in Nuclear Waste
PI: Dr. Dan Meisel *Institution:* University of Notre Dame

Description: This project, a collaborative ANL/PNNL effort, studies processes of the title system as it relates to the chemistry in high level liquid nuclear waste (HLW). The program is structured to transfer the information directly to the Hanford site operators (via “Organic Aging Studies, PI: Don Camaioni, PNNL). Our activity is also closely coordinated with another EMSP project (“Interfacial Radiolysis”, PI: Thom Orlando, PNNL) and we include below our results that relate directly to that project. We determined the redox potential of the NO32- radical and its possible conversion to NO radical rather than to NO2. We also determined the redox potential of the analogous NO22- radicals because this parameter will determine whether such a conversion is possible. We concluded that both NO2 and NO radicals are important intermediates in HLW and the relative importance will depend on the concentration of nitrite in the waste tank. As a consequence we will coordinate our activity with a recently awarded EMSP project that focuses on NO chemistry and its derivatives (“Reactivity of Peroxynitrite”, PI: Sergei Lymar, BNL).

Collaboration Type: Mission directed
Collaborator: Sergei Lymar, Thom Orlando
Collaborating Organization: BNL, Pacific Northwest National Laboratory

Project: 55264

Title: High Resolution Definition of Subsurface Heterogeneity for Understanding the Biodynamics of Natural Field Systems: Advancing the Ability for Scaling to Field Conditions
PI: Dr. Ernest L. Majer *Institution:* Lawrence Berkeley National Laboratory

Description: The objectives for this project were to develop and apply high-resolution seismic imaging methods for defining physical parameters (lithology, fracture content, fast paths, faults, etc.) that may be controlling flow and transport in naturally heterogeneous material. A primary aspect of the project was to determine if seismic imaging methods could resolve the details necessary to understand the physical heterogeneity controlling microbial behavior. Collaborations are with PNNL and INEEL. PNNL is collaborating in correlating the bacterial behavior to the zones of high permeability detected with the geophysics. INEEL provided the site (TAN) and drilling support as well as collaboration with other EMSP researchers (Colwell and Smith) in understanding the in-situ flow and microbial properties. There were also close collaborations with on site contractors (L. Peterson and T. Woods) in the collectionand processing of the data.

Collaboration Type: Consulting
Collaborator: Dr. Ardeth Simmons, LBL Yucca Mountain PM
Collaborating Organization: Yucca Mountain Project

Project: 55395

Title: Physics of DNAPL Migration and Remediation in the Presence of Heterogeneities

PI: Dr. Stephen H. Conrad *Institution:* Sandia National Laboratories

Description: For the Permanganate experiment, we worked with Dr. Jack Istok, a professor at Oregon State. Flushing with potassium permanganate has been investigated as an oxidizer that mineralizes TCE. Jack suspected that the manganese precipitate that forms as a mineralization product cause permeability reduction and thereby inhibit access between the TCE and the permanganate solution and this is precisely what we were able to visually observe in this experiment. The manganese precipitate formed a low permeability rind surrounding the DNAPL pools. Such results had not been seen previously, because for experiments run in uniform media, the DNAPL does not reside in pools. The permanganate oxidation process not likely to be as efficient as initially hoped in cases where DNAPL resides in pools. Perhaps intermittent flushes with a substance to dissolve away manganese precipitate might be possible.

Collaboration Type: Consulting
Collaborator: Dr. Jack Istok
Collaborating Organization: Oregon State

Description: The project involves conducting well-controlled laboratory experiments to better understand the physics of DNAPL migration and remediation in the presence of heterogeneities. The results will be used to test and to continue development of new modeling approaches. In addition, the results of the remediation experiments will be used to test the quantitative performance of remediation design codes within heterogeneous media. We intend to work closely with developers of each remediation approach to attempt to optimize the remedial process and show each technique in its best possible light. Towards that end, Alex Meyer, a professor at Michigan Tech, visited our lab and is collaborating with us on our first series of experiments looking at surfactant mobilization and solubilization of DNAPLs.

Collaboration Type: Consulting
Collaborator: Dr. Alex Meyer
Collaborating Organization: Michigan Tech

Description: For our MA surfactant experiment, we obtained surfactant advice from Alex Meyer and Lirong Zhong. The experiment used the surfactant MA and was designed to maximize solubilization while minimizing mobilization. Contrary to expectation, we observed dramatic mobilization. The DNAPL penetrated the aquitard and became inaccessible to the surfactant. Even though trapping number calculations predict some modest amount of mobilization, failure to account for DNAPL in pools resulted in significantly underestimating the potential for extensive downward mobilization. In observing the mobilization process, we discovered a previously unknown mobilization process that occurs when the surfactant front first encounters a pool. Very different interfacial tensions on either side of the surfactant front result in enhanced drainage of the DNAPL pool. For our particular experimental conditions, due to downward mobilization and penetration of the DNAPL into fine-grained units, introduction of the MA surfactant actually made the problem worse.

Collaboration Type: Consulting
Collaborator: Dr. Alex Meyer and Lirong Zhiong
Collaborating Organization: Michigan Tech

Description: For the Tween surfactant experiment, we obtained surfactant advice from Dr. Kurt Pennell, a professor at Georgia Tech. We obtained much better results using the Tween surfactant. We observed only modest DNAPL mobilization because the Tween surfactant maintains a much higher water/organic interfacial tension. We also observed good solubilization. Complete cleanup was achieved after several pore volumes of flushing. Time lapse animation of this experiment yielded important insights into remediation process.

Collaboration Type: Consulting
Collaborator: Dr. Kurt Pennell
Collaborating Organization: Georgia Tech

Description: We worked with Dr. Varadarajan Dwarakanath of Duke Engineering to design the tracer test. It occurred to us that the certain conditions provided by our remediation experiments – subsequent to the emplacement if the DNAPL and prior to beginning the remediation – were ideal for performing a tracer test while requiring very little extra work. Partitioning tracer tests are designed to compare the breakthrough of partitioning and non partitioning tracers. Retardation of the tracers that partition into the organic phase provides a means to calculate the mass of DNAPL contained in the region swept by the tracer test. We found that the test worked qualitatively, indicating the presence of DNAPL, but the calculations significantly underestimated the mass of DNAPL in the chamber. We believe that failure to account for the fact that the vast majority of the DNAPL mass existed in large pools resulted in under-prediction of DNAPL mass. When significant DNAPL mass exists in pools, typical tracer flow rates do not allow sufficient time for partitioning/diffusion of the tracers into and out of large pools.

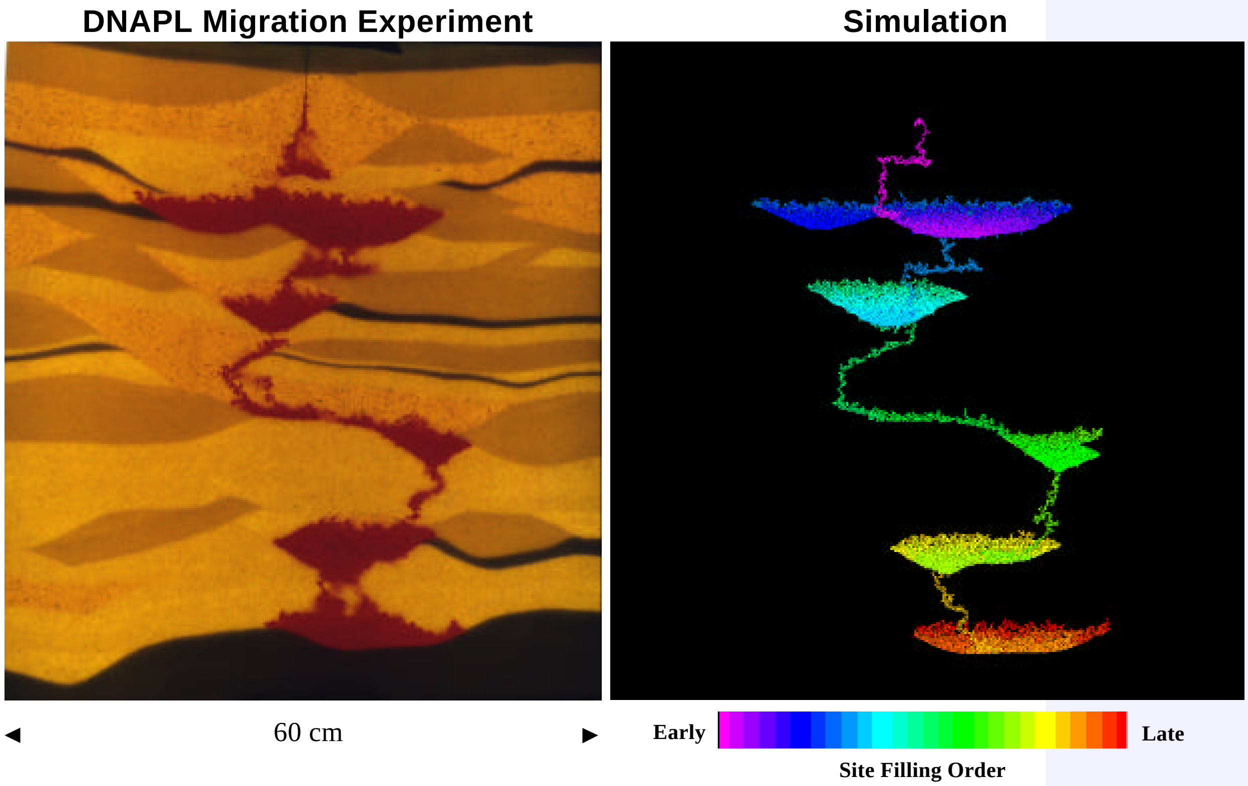
Collaboration Type: Consulting
Collaborator: Dr. Varadarajan Dwarakanath
Collaborating Organization: Duke Engineering

Project: 55410

Title: Determining Significant Endpoints for Ecological Risk Analysis
PI: Dr. Thomas G. Hinton *Institution:* Savannah River Ecology Laboratory

Description: The PI has taken knowledge gained from this research and used it in his work with the DOE Biota Dose Assessment Group (BDAG). BDAG is currently reviewing ecological risk concepts and establishing guidelines for conducting ecological risks on DOE Facilities.

Collaboration Type: Consulting
Collaborator: Dr. Thomas Hinton
Collaborating Organization: Savannah River Ecology Lab - University of Georgia



Results of a DNAPL migration experiment conducted at Sandia National Laboratories are compared to upscaled percolation modeling. The photo (left) illustrates that the DNAPL(dyed red) migrated downward due to its high density but that aquifer heterogeneities caused significant pooling along the migration path. DNAPL in such a configuration served as the initial condition for remediation experiments. The simulation image (right) compares extremely well with the experiment. [see Project #55395]

Project: 55416

Title: Control of Biologically Active Degradation Zones by Vertical Heterogeneity: Applications in Fractured Media

PI: Dr. Frederick S. Colwell *Institution:* Idaho National Engineering and Environ-mental

Description: The DOE is faced with cleaning up wastes from reactor and weapons production activities during the last fifty years. Many DOE sites have contaminants that are difficult to access due to depth and complex geology and are challenging to degrade using conventional methods. The key objective of this project is to determine the distribution of biologically active contaminant degradation zones in a fractured, subsurface medium with respect to vertical heterogeneities.

Collaboration Type: Consulting

Collaborator: Lance Peterson, Kent Sorenson, and Joe Rothermel

Collaborating Organization: Idaho National Engineering and Environmental Laboratory; Parsons

Project: 59849

Title: Radionuclide Immobilization in the Phases Formed by Corrosion of Spent Nuclear Fuel: The Long-Term Assessment

PI: Dr. Rodney C. Ewing *Institution:* University of Michigan

Description: Continued efforts to evaluate the capabilities of the uranyl phases to incorporate and retard release of important radionuclides: Np-237, Se-79, Tc-99, and I-129.

Collaboration Type: Program interaction

Collaborator: Professor Peter Burns

Collaborating Organization: Notre Dame

Project: 59882

Title: Measurements of Radon, Thoron, Isotopic Uranium and Thorium to Determine Occupational & Environmental Exposure & Risk at Fernald Feed Materials Production Center.

PI: Dr. Naomi H. Harley *Institution:* New York University Medical School

Description: Dr. Fisenne at USDOE Environmental Measurements Laboratory has developed a sequential radiochemical procedure to analyze any environmental sample matrix, presently focused on Soil samples, for Lead-210, radium, thorium, and uranium isotopes

Collaboration Type: Consulting

Collaborator: Dr. Isabel Fisenne

Collaborating Organization: Environmental Measurements Laboratory

Project: 59918

Title: Improved Radiation Dosimetry/Risk Estimates to Facilitate Environmental Management of Plutonium Contaminated Sites

PI: Dr. Bobby R. Scott *Institution:* Lovelace Biomedical & Environmental Research

Description: Additional data on lung cancer induced in Mayak workers exposed by inhalation to both plutonium and cigarette smoke were acquired by Dr. Scott from scientists at the Branch No. 1 of the Institute of Biophysics, Ozersk Russia. The data will facilitate making conclusions about possible interactions between alpha radiation and cigarette smoke in the induction of lung cancer. The data will also allow for additional insights to be made related to the validity of the linear, no-threshold hypothesis for cancer induction

Collaboration Type: Mission directed

Collaborator: Unknown

Collaborating Organization: Branch No. 1 of the Institute of Biophysics, Ozersk Russia

Description: We are now assisting staff at the Rocky Mountain Remediation Services, L.L.C., Rocky Flats Environmental Technology Site in preparing a scientifically valid approach to selecting respiratory protection devices for use in very high concentrations of plutonium. Some concentration of interest would essentially lead to early occurring or delayed deaths without adequate worker protection. The activities at Rock Flats relate to decontamination and decommissioning. Our staff reviewed an original draft white paper related to selecting appropriate respiratory devices and major shortcomings related to protecting DOE decontamination/decommissioning workers were pointed out. We will continue to assist in preparing a more credible plan for protecting workers and in preparing an associated white paper

Collaboration Type: Consulting
Collaborator: Rocky Mountain Remediation Services, L.L.C.,
Collaborating Organization: Rocky Flats Environmental Technology Site

Project: 59960

Title: Direct Investigations of the Immobilization of Radionuclides in the Alteration Phases of Spent Nuclear Fuel
PI: Dr. Peter C. Burns *Institution:* University of Notre Dame

Description: The NSNFP is interested in this research concerning the mobility of the radionuclides in SNF for their work on the repository at Yucca Mtn. Dr. Burns is collaborating with ANL-E, where they are performing drip tests in a hot cell on commercial SNF. Ms. Davis has a work package funded by the NSNFP which funds ANL-E to perform similar release rate testing on DOE SNF. She is interested in having Dr. Burns perform an analysis on DOE SNF, similar to what he has done on commercial SNF. Dr. Paul Lessing is investigating the incorporation of Gadolinium as a neutron absorber into the DOE SNF packages which will be sent to Yucca Mtn. He would be interested in having Dr. Burns investigate the mobility of Gd in SNF packages.

Collaboration Type: Mission directed
Collaborator: Colleen Shelton-Davis
Collaborating Organization: National Spent Nuclear Fuels Program

Description: Solved the crystal structure of a novel uranyl silicate formed during the corrosion of an actinide-bearing waste glass.

Collaboration Type: Program interaction
Collaborator: Rudolph Olson
Collaborating Organization: Argonne National Laboratory

Project: 60020

Title: Stability of High-Level Waste Forms
PI: Dr. Theodore M. Besmann *Institution:* Oak Ridge National Laboratory

Description: Experimental studies of phase relations in the sodium oxide-boron oxide-uranium (VI) oxide system are being run in this EMSP program because there is no information in the literature. This data is needed for modeling actinide behavior in glasses. The results of these tests are also being spun off to assist the Uranium-233 Disposition Program of the Office of Fissile Materials Disposition (DOE/MD). They are considering dissolution of uranium oxide in sodium borate or boron oxide as an option for Uranium-233 disposition. As experimental data is produced, it is made available to the Uranium-233 Program to assist in their development of a flow sheet. Because of the dearth of information on this system, it is not surprising that any information that is produced may be applied in different activities.

Collaboration Type: Joint interaction
Collaborator: Charles Forsberg
Collaborating Organization: Oak Ridge National Laboratory

Description: Models of phase relations and liquidus temperatures developed in this EMSP program are being used to evaluate test results from the Tanks Focus Area Immobilization Program "Waste Loading Improvements in High and Low Activity Glasses and Waste Form Product Acceptance Testing." The focus at this time is on conditions where crystallization occurs in glass processing. By applying models to the test data, an understanding of crystallization and how to avoid it may be obtained.

Collaboration Type: Joint interaction
Collaborator: John Vienna
Collaborating Organization: Pacific Northwest National Laboratory

Project: 60069

Title: Least-Cost Groundwater Remediation Design Using Uncertain Hydrogeological Information

PI: Dr. George F. Pinder *Institution:* University of Vermont

Description: The project seeks to examine the importance of uncertainty in hydraulic conductivity in the least-cost design of groundwater contamination containment systems. The project uses a new conceptual approach to accommodate aquifer parameter uncertainty in optimal groundwater remediation design and introduces a new operations-research technique to solve the optimization problem. The new approach, Robust Optimization, allows for the determination of a robust, lowest-possible cost, pumping design that is consistent with the inherent uncertainty in the hydraulic conductivity field. It also allows for the visualization of how one can trade off excess pumping for enhanced security. Collaborated with BNL for a review of Brookhaven groundwater contamination.

Collaboration Type: Consulting
Collaborator:
Collaborating Organization: Brookhaven National Laboratory

Project: 60075

Title: Particle Generation by Laser Ablation in Support of Chemical Analysis of High Level Mixed Waste from Plutonium Production Operations
PI: Dr. J. Thomas Dickinson *Institution:* Washington State University

Description: Performing laser ablation/description analytical determination on a surrogate sample. Contacted Arlin Olson and Scott Herbst to identify the surrogate and analytical requirements. Investigate analysis of these samples by laser ablation IMP-MS as well as a related method, laser desorption mass spectroscopy to determine key molecular components. The goal is to generate a complete mass balance of the calcine waste
Collaboration Type: Joint interaction
Collaborator: Jim Rindfleisch
Collaborating Organization: Long Range Waste Management Program, Idaho National Engineering and Enviornmental Laboratory

Description: We have been working with Dr. Beverly Crawford. Dr. Crawford is in charge of a laser ablation ICP-MS system that has been installed in a hot cell in the Hanford 222S building. One of the key technical questions is how well laser ablation can determine the overall bulk composition of a heterogeneous sample given a small volume of material sampled. We have begun to address the homogeneity issue .
Collaboration Type: Joint interaction
Collaborator: Dr. Beverly Crawford
Collaborating Organization: Numatec, Hanford

Project: 60118

Title: Fundamental Thermodynamics of Actinide-Bearing Mineral Waste Forms
PI: Dr. Mark A. Williamson *Institution:* Los Alamos National Laboratory

Description: The end of the Cold War raised the need for the technical community to be concerned with the disposition of excess nuclear weapon material. The plutonium will either be converted into mixed-oxide fuel for use in nuclear reactors or immobilized in glass or ceramic waste forms and placed in a repository. The stability and behavior of plutonium in the ceramic materials as well as the phase behavior and stability of the ceramic material in the environment is not well established. The purpose of this project is to determine the thermodynamic data essential to developing an understanding of the chemistry and phase equilibria of the waste form materials proposed as immobilization matrices. Collaboration with DOE-MD program for Dispositioning of Plutonium by
Collaboration Type: Program interaction
Collaborator:
Collaborating Organization: DOE-Office of Fissile Materials Disposition

Project: 60283

Title: Waste Volume Reduction Using Surface Characterization and Decontamination by Laser Ablation

PI: Dr. Michael J. Pellin *Institution:* Argonne National Laboratory

Description: The waste stream generated in the D&D efforts for nuclear facilities includes a significant volume of material that is contaminated only in the surface or near-surface region. It is critical to understand the depth-dependent concentration and chemistry of radionuclide-contaminated surfaces. Complete removal and capture of the contaminated surface would greatly reduce the volume of waste material generated in, and thus the cost of, D&D efforts. This project represents the first detailed surface studies of the sorption of radionuclides in complex materials such as concrete. Collaboration is a joint interaction with Zawtech Inc. to do further research into areas of practical applications

Collaboration Type: Joint interaction

Collaborator:

Collaborating Organization: Zawtech Inc.

Project: 60296

Title: Research Program to Investigate the Fundamental Chemistry of Technetium

PI: Dr. Norman M. Edelstein *Institution:* Lawrence Berkeley National Laboratory

Description: This project addresses the fundamental solution chemistry of technetium (Tc) in the waste tank environment, and the stability of Tc in various waste forms. A separate facet of this project is the search for lower valent forms of Tc that may be incorporated in various waste forms for long term storage. Collaborated with PNNL as a participant (technical expert) at Technetium Chemistry workshop review panel assessing tank technetium removal/disposition options.

Collaboration Type: Consulting

Collaborator:

Collaborating Organization: Pacific Northwest National Laboratory

Project: 60362

Title: Ion-Exchange Processes and Mechanisms in Glasses

PI: Dr. B. Peter McGrail *Institution:* Pacific Northwest National Laboratory

Description: The objective of this project is to develop an understanding of the processes and mechanisms controlling alkali ion exchange and to correlate the kinetics of the ion-exchange reaction with glass structural properties. The fundamental understanding of the ion-exchange process developed under this study will provide a sound scientific basis for formulating low exchange rate glasses with higher waste loading, resulting in substantial production and disposal cost savings. Collaboration with Dr. David K. Shuh at the Lawrence Berkeley National Laboratory

Collaboration Type: Program interaction
Collaborator: D.K. Shuh
Collaborating Organization:

Project: 60403

Title: Phase Chemistry of Tank Sludge Residual Components
PI: Dr. James L. Krumhansl *Institution:* Sandia National Laboratories

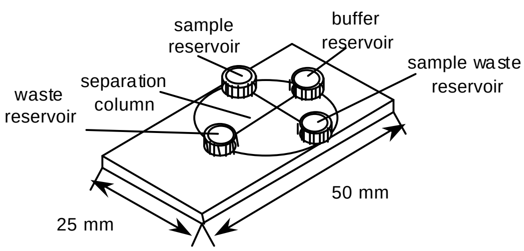
Description: Because it is not possible to recover all of the contaminated sludge from the bottoms of decommissioned waste storage tanks, a credible model for the release of radionuclides from residual sludge is needed. Those sludge components most likely to retain radionuclides will be identified and synthesized. Radionuclide sorption and desorption will also be studied. AFM and STM studies will provide a firm atomistic explanation for the observed interactions between the sludge, solutions, and radionuclides. This understanding will be used to develop a quantitative radionuclide release source term for use in the performance assessment calculations. Collaboration with Larry Bustard at TFA regarding aspects of tank fluid/sludge interactions.
Collaboration Type: Consulting
Collaborator: Larry Bustard
Collaborating Organization: TFA

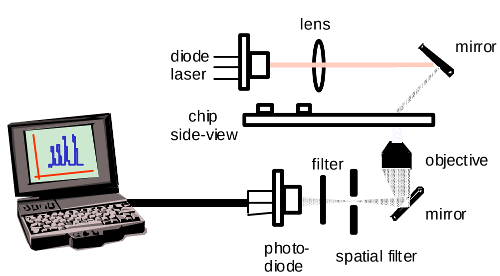
Project: 64982

Title: Metal Ion Analysis Using Near-Infrared Dyes and the “Laboratory-on-a-Chip”
PI: Dr. Greg E. Collins *Institution:* Naval Research Laboratory

“Laboratory-on-a-Chip”

Instrumentation





J.M. Ramsey et. al., AnalChem, 67, 2059 (1995).

The Laboratory-on-a-Chip is intended to provide a field portable characterization instrument for in-situ waste characterization. [see Project #64982]

Description: This project addresses the need for developing a new class of radionuclide and heavy metal complexation agents that are tagged with near-infrared dyes and, therefore, can be extended to the implementation of a compact and portable "laboratory-on-a-chip" operable in the stringent field requirements of DOE site characterization and remediation. Collaboration with Dick Meservey with the Decontamination and Deactivation Focus Area to refine the project direction. Commitments to support field-testing have been

Collaboration Type: Mission directed

Collaborator: Dick Meservey

Collaborating Organization: DDFA

Project: 65411

Title: Precipitation and Deposition of Aluminum-Containing Phases in Tank Wastes

PI: Dr. Jun Liu *Institution:* Pacific Northwest National Laboratory

Description: Aluminum-containing phases represent the most prevalent solids that can appear or disappear during the processing of radioactive tank wastes. Of all constituents of tank waste, Al-species have the greatest potential for clogging pipes and transfer lines, fouling highly radioactive components such as ion exchangers, and completely shutting down processing operations. The primary focus of this project is to understand the major factors controlling precipitation, scale formation, and cementation of existing soluble particles by Al-containing phases. The results will be used to predict and control precipitation, scale formation, and cementation under tank waste processing conditions. The results will also provide information regarding what Al-containing phases form and how soluble such phases are in basic tank waste solutions. The project will have an important impact on waste minimization and on the retrieval, transport, and separation of tank wastes. Collaboration with Dr. Albert Hu at Lockheed Martin Hanford Company to perform simulations to support the ESP modeling work at Hanford.

Collaboration Type: Program interaction

Collaborator: Dr. Albert Hu

Collaborating Organization: Lockheed Martin Hanford Company

Project: 65435

Title: Millimeter-Wave Measurements of High Level and Low Activity Glass Melts

PI: Dr. Paul P. Woskov *Institution:* Massachusetts Institute of Technology

Description: The objectives of the project are to develop new real-time sensors for characterizing glass melts in high level waste (HLW) and low activity waste (LAW) melters, and to understand the scientific basis and bridge the gap between glass melt model data and melter performance. A basic goal is to characterize glass melts in-situ with the new diagnostic capability so that data will represent the actual melt's behavior. The work will be closely coupled to the needs of the Defense Waste Processing Facility, West Valley Demonstration Project, and vitrification efforts at Hanford, Oakridge, and Idaho sites. The project is a collaboration between the MIT Plasma Science and Fusion Center, PNNL, and the Savannah River Technology Center. In addition, discussions are in progress with Tom Thomas of the Tanks Focus Area regarding the possibility of demonstrating with the TFA.

Collaboration Type: Program interaction
Collaborator: Tom Thomas
Collaborating Organization: Tanks Focus Area

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